

Supplementary data

Hg₂Ru₂O₇, a new pyrochlore showing a metal/insulator transition

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Observed and calculated X-ray powder diffraction data for Hg₂Ru₂O₇ at 293 K with d > 0.89 Å (Cu K α_1 radiation)

No.	observed			h k l			calculated		
	d	2 θ	I _{rel}	d	2 θ	I _{rel}	d	2 θ	I _{rel}
1	5.8946	15.018	8.0	1	1	1	5.8896	15.030	6.48
2	3.0762	29.003	5.5	3	1	1	3.0758	29.007	4.17
3	2.9452	30.323	100.0	2	2	2	2.9448	30.327	100.0
4	2.5505	35.159	37.3	4	0	0	2.5503	35.161	36.16
5	2.3404	38.433	9.2	3	3	1	2.3403	38.434	7.24
6	2.0824	43.421	0.3	4	2	2	2.0823	43.422	0.24
7	1.9631	46.205	3.6	5	1	1	1.9632	46.204	3.06
8	1.8033	50.576	40.6	4	4	0	1.8033	50.574	39.54
9	1.7243	53.070	2.8	5	3	1	1.7243	53.068	2.41
10	1.6121	57.087	0.2	6	2	0	1.6129	57.054	0.19
11	1.5556	59.362	0.5	5	3	3	1.5557	59.360	0.41
12	1.5378	60.120	34.7	6	2	2	1.5379	60.117	38.27
13	1.4724	63.090	9.0	4	4	4	1.4724	63.088	10.08
14	1.4284	65.267	0.9	7	1	1	1.4284	65.266	0.89
15	1.3280	70.904	0.9	7	3	1	1.3281	70.902	0.95
16	1.2751	74.328	4.1	8	0	0	1.2751	74.326	5.42
17	1.2462	76.357	0.7	7	3	3	1.2463	76.353	0.84

Supplementary Material (ESI) for *Journal of Materials Chemistry*
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18	1.1779	81.684	0.7	7	5	1	1.1779	81.679	0.83
19	1.1701	82.342	10.1	6	6	2	1.1702	82.339	14.08
20	1.1405	84.972	8.1	8	4	0	1.1405	84.969	12.32
21	1.1197	86.935	0.6	9	1	1	1.1197	86.934	0.87
22	1.0694	92.158	0.2	9	3	1	1.0694	92.163	0.24
23	1.0411	95.438	5.5	8	4	4	1.0412	95.438	9.76
24	1.0252	97.411	0.4	7	7	1	1.0253	97.410	0.74
25	0.9862	102.721	0.2	9	5	1	0.9862	102.721	0.42
26	0.9816	103.390	5.3	10	2	2	0.9816	103.392	11.67
27	0.9513	108.145	0.2	9	5	3	0.9513	108.146	0.34
28	0.9199	113.729	0.2	11	1	1	0.9198	113.745	0.29
29	0.9017	117.364	1.4	8	8	0	0.9017	117.367	3.94
30	0.8913	119.597	0.2	11	3	1	0.8913	119.597	0.69
